ATBD for the MSG GII/TOZ Product

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1 INTRODUCTION

1.1 Purpose of this Document

This document describes the algorithm theoretical basis for the derivation of the Global Instability Indices (GII) product, as it shall be derived from the Meteosat Second Generation SEVIRI instrument (MSG-SEVIRI). The GII derivation also includes the derivation of the total column ozone product (TOZ), i.e. the TOZ retrieval scheme is also described in this document.

1.2 Structure of this Document

Section 2 of this document provides a short overview over the MSG-SEVIRI instrument characteristics. This is followed by a detailed description of the underlying algorithm of the GII/TOZ product – its physical basis, the required input data, and a more detailed description of the product retrieval method.

At the end, relevant literature references are provided.

2 OVERVIEW

2.1 Relevant Instrument Characteristics

The mission of the Meteosat Second Generation (MSG) System is to provide continuous high spatial, spectral and temporal resolution observations and geophysical parameters of the Earth / Atmosphere System derived from direct measurements of its emitted and reflected radiation using satellite based sensors from the geo-stationary orbit.

The meteorological products described in this document will be extracted from the data of the Spinning Enhanced Visible and Infrared Radiometer (SEVIRI) mission. SEVIRI scans the full disc in 15 minutes, and can also be operated in a rapid scan service to cover parts of the disk in accordingly shorter time intervals.

SEVIRI acquires the spectral channels simultaneously by scanning three rows of detectors per spectral channel in an east/west direction to form three consecutive image lines. Subsequent image lines are collected moving from south to north to form an image per spectral channel covering either the full disc coverage or the rapid scan service coverage within the respective repeat cycle duration. Radiance samples are created from the detector elements at specific spatial sample locations and are then rectified to a reference grid, before dissemination to the End Users as Level 1.5 datasets.

Table 1: Channel specification for the MSG-SEVIRI Instrument

Spectral Channel	*Central Wavelength*	*Range*	*Spatial Sampling Distance (SSD)*
VIS 0.6	0.635 µm	0.56 – 0.71 µm	3.0 km
VIS 0.8	0.810 µm	0.74 – 0.88 µm	3.0 km
NIR 1.6	1.600 µm	1.50 – 1.78 µm	3.0 km
IR 3.9	3.920 µm	3.48 – 4.36 µm	3.0 km
WV 6.2	6.325 µm	5.35 – 7.15 µm	3.0 km
WV 7.3	7.350 µm	6.85 – 7.85 µm	3.0 km
IR 8.7	8.700 µm	8.30 – 9.10 µm	3.0 km
IR 9.7	9.660 µm	9.38 – 9.94 µm	3.0 km
IR 10.8	10.800 µm	9.80 – 11.80 µm	3.0 km
IR 12.0	12.000 µm	11.00 – 13.00 µm	3.0 km
IR 13.4	13.400 µm	12.40 – 14.40 µm	3.0 km
HRV	-	0.5 – 0.9 µm	1.0 km

3 ALGORITHM DESCRIPTION

3.1 Physical Basis Overview

Instability parameters are derived from vertical profiles of temperature and humidity to provide some information concerning the vertical stability of the atmosphere. Various indices are used by forecasters for different applications and regions, and these indices are defined as a difference of profile parameters in different pressure levels (Galway, 1956, Kurz, 1993). Such data are usually derived from radio soundings, but a few satellite derived indices also exist (e.g. derived from the GOES satellites, e.g. Hayden, 1988, Rao and Fuelberg, 1997). The air mass parameters can be used to issue severe weather warnings if the corresponding index exceeds a certain threshold. These thresholds are usually determined empirically and should not be regarded as fixed values – they may vary from season to season and from region to region. A skilled local forecaster is absolutely necessary for a correct interpretation of the provided indices.

The chosen GII retrieval scheme also implicitly includes the retrieval of layer precipitable water and total column ozone, which are also described in this document.

The combined GII/TOZ (for simplicity hereafter only referred to as the GII product) will comprise the following instability indices, other air mass parameters relevant to atmospheric stability and ozone values:

- Lifted Index $LI = T - T^{\text{lifted from surface}}$ at 500 hPa
- K-index $KI = (T^{(850)} - T^{(500)}) + TD^{(850)} - (T^{(700)} - TD^{(700)})$
- KO-index $KO = 0.5\,(\Theta_e^{(500)} + \Theta_e^{(700)} - \Theta_e^{(850)} - \Theta_e^{(1000)})$
- Maximum Buoyancy $MB = \Theta_e^{max} - \Theta_e^{min}$
- Layer Precipitable Water, (humidity, vertically integrated over three different layers)
- Total Precipitable Water, (humidity, vertically integrated over the entire atmosphere)
- Total Column Ozone (TOZ), (ozone, vertically integrated over the entire atmosphere)

where

T is the air temperature at the indicated pressure level (e.g. T(850) is at 850 hPa), expressed in Kelvin
TD is the dew point temperature, expressed in Kelvin, again at the indicated pressure level
Θ_e is the equivalent potential temperature, at the indicated pressure level
Θ_e^{max} is the maximum Θ_e between the surface an 850 hPa
Θ_e^{min} is the minimum Θ_e between the 700 and 300 hPa
Humidity refers to the atmospheric water vapour content expressed as mixing ratio q, expressed in kg/kg or ppmv
Ozone refers to the atmospheric ozone content, expressed as mixing ratio, expressed in kg/kg or ppmv
The *Layer* and *Total Precipitable Water* are expressed as kg/m^2, *Total Colum Ozone* in Dobson Units

The main purpose of the algorithm is to retrieve a profile of atmospheric temperature, humidity and ozone, from which the above parameters can be derived. The chosen algorithm approach is a so-called statistical-physical retrieval in that prior information and measurements are combined in a statistically optimal way, with a physical radiative transfer model used to relate atmospheric properties to measurements. Prior information is required because the information contained in the observed radiances is not sufficient to completely define the atmospheric profile. The prior profile (also known as “background profile”) is obtained from short range NWP forecasts and also serves as the “first guess” profile. The solution will contain information of these forecasts and will not be completely independent of the forecast. During the retrieval, the profile is adjusted such that the statistical likelihood of the profile is maximised, or – equivalently – the solution cost is “minimised. Within the GII processing, this minimisation is assumed achieved when simulated radiances match observed values to within a pre-determined threshold.

Effectively the method infers temperature, humidity and ozone profiles from observed radiances in a given set of channels and given (usually NWP forecast) atmospheric profiles. The air mass parameters are then derived from the resulting profiles. The physical retrieval is an optimal estimation using an inversion technique, i.e. tries to find an atmospheric profile which best reproduces the observations (Rodgers, 1976). In general, this is a multi-solution problem, and a “background profile” is used as a constraint. This background profile is often also referred to as “first guess”, as it is fed to the iteration scheme as an initial proposal for a solution. The original first guess is then slowly modified in a controlled manner until its radiative properties fit the satellite observations. A typical first guess field is a short-term forecast. The final profile is the profile where the simulated radiance field at the top of the atmosphere matches the satellite observations, or in practice, until its difference to the observations is minimal.

The core of the retrieval is the profile adjustment step (Ma et al. 1999, or Rodgers, 1976):

$$x_{n+1} = x_0 + (\mathbf{S}_x^{-1} + \mathbf{K}_n^T \cdot \mathbf{S}_\varepsilon^{-1} \cdot \mathbf{K}_n)^{-1} \times \mathbf{K}_n^T \cdot \mathbf{S}_\varepsilon^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0)\right] \qquad \textbf{(1)}$$

with

- x: state vector (atmospheric profile, together with a lower boundary condition)
- n: iteration step, n=0 denotes background profile
- T_B: observed brightness temperatures
- $T_{B,n}$: simulated brightness temperatures for profile of iteration step n
- $\mathbf{S}_x$: error covariance matrix of background
- $\mathbf{K}_n$: Jacobian matrix at iteration step n
- $\mathbf{S}_\varepsilon$: error covariance matrix of observed brightness temperatures and of the radiation model

Sections 3.4 and 3.5 provide a detailed description of each term in the retrieval equation.

Equation (1) describes the iterative method of solution; the iteration process is stopped if the difference in observed and simulated brightness temperatures is small (for details, see section 3.5.2).

Furthermore, equation (1) implies that the physical retrieval needs a model for the radiative forward and Jacobian calculations, i.e. the model has to be capable to simulate brightness temperatures in the MSG channels of interest for a specific atmospheric profile and viewing geometry, and for the same case has to provide the partial derivates $\partial T_B/\partial x(i)$ (change of simulated brightness temperature due to a change in the vertical profile x at level i), i.e. the Jacobians K in equation (1). The model RTTOV provided by the EUMETSAT NWP-SAF (Satellite Application Facility for Numerical Weather Prediction) has this functionality. RTTOV uses a set of M fixed pressure levels between the surface and the top of the atmosphere (e.g. 0.1 hPa), so that the profile data will in the end be available on this vertical grid.

Two versions of this retrieval will be described in this document:

3.1.1 Version I – Cloud Free Conditions, Full GII/TOZ Retrieval

This version is only applicable to clear sky conditions. In this case the full set of relevant MSG-SEVIRI channel information will be explored, and the first guess temperature, humidity, and ozone profile may be changed within the retrieval. The relevant lower boundary condition is the surface skin temperature (which may also be changed by the retrieval).

All instability and airmass parameters and the total column ozone can be derived from the final profile information. Details are provided in section 3.5.6. Details on how to terminate the iteration process are provided in section 3.5.2.

3.1.2 Version II – Cloudy Conditions, TOZ Retrieval

Theoretical considerations concerning the information content of the MSG IR 9.7 channel (the ozone channel), together with the fact that most of the atmospheric ozone is in the stratosphere, showed that a meaningful retrieval of total column ozone is possible over low clouds. For this special case, the lower boundary condition needs to be changed to the cloud top pressure. With respect to the atmospheric profile, only the ozone profile is subject to changes within the retrieval.

The total column ozone can then be derived from the final profile information. Details on how to terminate the iteration process are provided in section 3.5.2.

3.2 Assumptions and Limitations

As outlined in the previous section, a meaningful full GII/TOZ processing is only possible for clear sky conditions, only the TOZ product can also be retrieved over low clouds.

An important underlying assumption of the process is that the retrieved (assumed to be the "true") profile is not too much different from the background profile, i.e. from the forecast. The spectral information content of the MSG IR channels is certainly not high enough to derive a forecast independent atmospheric profile, i.e. for MSG-SEVIRI many solutions for equation (1) exist and could theoretically be found. Usage of the forecast as background constrains the problem to the solution which is closest to the forecast, meaning that the final solution will retain certain features of the background. Validation work, also based on the MSG-SEVIRI GII product, however, has shown that this is in practice fully sufficient and acceptable (Koenig and de Coning, 2010).

3.3 Algorithm Basis Overview

The core of the GII algorithm is to solve the retrieval equation (1). The processing is done on the level of an individual image pixel or a group of pixels, e.g. defined as a box of pixels. The basic processing element will hereafter be referred to as Field-of-Regard (FoR).

For each FoR, necessary input data need to be prepared (see section 3.4). The iterative retrieval is schematically shown in Figure 1. Specific details on all the processing steps are provided in section 3.5, also with focus on the two different versions A and B.

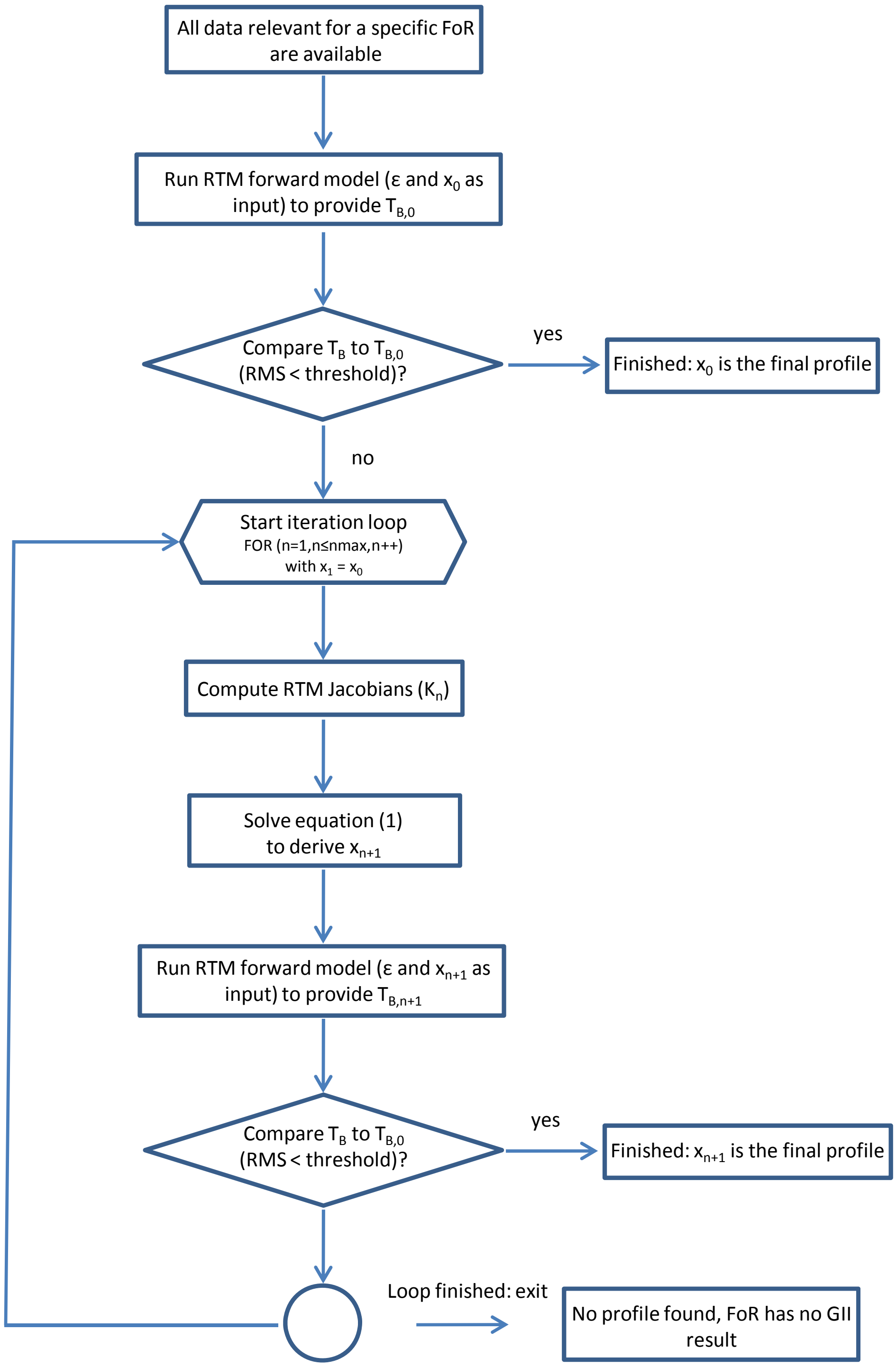

Figure 1: Schematic flow diagram for the GII/TOZ processing for a given FoR

3.4 Algorithm Input

Table 2 lists the data that needs to be available before the start of the GII processing.

Table 2: Necessary input data for the GII processing

Parameter Description	Variable Name
Brightness Temperatures for the L=7 MSG-SEVIRI channels WV 6.2, WV 7.3, IR 8.7, IR 9.7, IR 10.8, IR 12.0, IR 13.4, for each pixel within the processing area	$T_B(ch)$
Bias corrections for the seven MSG-SEVIRI channels	$T_{bias}(ch)$
Satellite viewing angles for each pixel within the processing area	ζ_{sat}
Surface emissivity information, for the seven channels, for each pixel over the processing area	$\varepsilon(ch)$
ECMWF[1] profiles of temperature, humidity, ozone, surface skin temperature for the processing area, on the M vertical levels of RTTOV, for two forecast times bracketing the image time	$T(p)$, $q(p)$, $o_3(p)$, T_{skin} - all combined in vector x_0
Surface type information for the ECMWF[1] grid points within the processing area (land or sea)	SType
Results of the Cloud Mask Product, for each pixel within the processing area; underlying surface type for clear sky (land/sea)	SCE
Observation and radiative transfer model error matrix	$\mathbf{S}_\varepsilon$
Error Covariance Matrix of background	$\mathbf{S}_x$

[1]: ECMWF = European Centre for Medium Range Weather Forecasts

3.4.1 Primary Sensor Data

For each FoR, the brightness temperatures in L=7 MSG-SEVIRI channels, as listed in Table 2, must be available. The availability of this data goes together with the Cloud Mask Product CM, which is also a pixel based product, defined on the same IR grid as the IR channels.

For the case that the FoR is larger than a single MSG IR pixel (e.g. a box of pixels), the brightness temperatures need to be averaged over this area. This averaging has to be done separately for the cloudy and cloud free pixels, as described by the SCE product oputput. This will result in average brightness temperatures for the cloud free section of the box, and in average brightness temperatures for the cloudy section of the box (obviously accounting for the fact that the entire box may be cloud free or cloud filled). The decision on which retrieval version (I or II) to select, is based on the number of cloud free pixels:

If more than 50% of the FoR is cloud free, the Version I is selected, using the average cloud free brightness temperatures. If more than 50% of the FoR, however, are cloudy, Version II is selected, using the average cloudy brightness temperatures.

Note: An absolutely correct average should use the original radiances as input, i.e. derive an average radiance, and then convert this radiance to the average temperature. Simulations, however, have shown that the differences are negligible, so that the averaging can be safely done in brightness temperature space.

For the case that the FoR is just a single pixel, the decision is simply based on this pixel's cloud product: If the pixel is declared cloud free, Version I is selected, if it is cloudy, Version II shall be selected.

After having identified the correct (average) brightness temperatures for the given FoR, measurements are bias corrected. Such a correction accounts for the (possible) bias between the satellite and the radiation model and model forecasts. Such biases must be assessed in an independent step, e.g. by the bias monitoring which is routinely done at ECMWF. For all L channels, the bias is defined such that for each channel a fixed value is added to the original brightness temperature.

$$T_B(ch) = T_{B,observed}(ch) + T_{bias}(ch) \qquad \textbf{(2)}$$

$T_{B,observed}$: observed brightness temperature for a given position
T_{bias}: bias correction term
ch: index for channel

The thus defined corrected brightness temperatures are the T_B values specified in equation (1).

3.4.2 Ancillary Dynamic Data

3.4.2.1 Cloud Mask Product (SCE)

As already described in section 3.4.1, the Cloud Mask Product (taken from the Scenes Analysis SCE) needs to be available for the correct preparation of the FoR's brightness temperatures. This cloud mask is available on a pixel basis (of the IR channel resolution). The SCE product takes the value "cloudy", "cloud free" or "unknown" – pixels with an "unknown" cloud mask shall be disregarded for the GII processing.

3.4.2.2 Forecast Data

The other important ancillary dynamic dataset are the forecast profiles of temperature, humidity and ozone, denoted as the x_0 background profile in equation (1). Within the GII processing, the x_0 background profile is also taken as the first guess, i.e. as input to the first run of the radiative forward model to derive the simulated brightness temperatures $T_{B,0}$. Since the RTTOV radiation model is used for the radiative transfer calculations, the profile parameters are represented at a maximum of M levels (M is defined within RTTOV, e.g. for RTTOV-9.1 M=43). The radiation model needs the profile parameters at M prescribed pressure levels so that the background profile must be appropriately interpolated to these levels (logarithmic interpolation for temperature, linear interpolation for humidity and ozone, all with respect to pressure). The level 1 is assumed to be at the top of the atmosphere, level M is at the surface.

The profile information is taken from the ECMWF forecast data, which is defined on a specific latitude/longitude grid. Each profile is interpolated both in space and time to fit the time and location of the actual satellite observation. As a surface value, the ECMWF forecasted skin temperature – also appropriately interpolated - is used in the retrieval as the temperature of the lowest layer. The observation vector thus has a length of 3M+1, i.e. M temperature values T, M humidity values q, M ozone values o_3 and the surface skin temperature T_{skin} (in this order). All temperatures are expressed in unit Kelvin, the humidity and ozone are expressed as ppmv. The pressure levels p are prescribed by RTTOV and are given in hPa.

In case the actual surface pressure is smaller than the lowest RTTOV level (e.g. 1013.25 hPa), the RTTOV levels between the lowest level and the first level above the actual surface shall be simply populated with the temperature, humidity and ozone value of the lowest model level.

In case of the special Version II processing the lower boundary condition is changed from the surface skin temperature to the cloud top pressure. The background cloud pressure (entry for x_0) is set to 882.8 hPa (or to the RTTOV prescribed pressure level in the vicinity of this value), the first guess cloud top pressure, however, is the pressure level, where

$$\left| T_B(\mathrm{channel\,IR10.8}) - T_{B,\mathrm{overcast}}(\mathrm{IR10.8}, p) \right|$$

is minimal. T_B(channel IR 10.8) is the measured and bias corrected temperature in channel IR 10.8, $T_{B,overcast}$(IR10.8,p) is the simulated brightness temperature in channel IR 10.8 for a cloud at pressure p. The $T_{B,overcast}$ results are one of the outputs of RTTOV, at each of the M pressure levels.

Within the spatial interpolation of the ECMWF profiles, care has to be given to the actual surface type value of the forecast points compared to the (predominant) surface type of the FoR. Only those ECMWF grid points, which have the same surface type (only land/sea are discriminated), shall be used for the spatial interpolation.

If, for example, a specific FoR has surface type “land”, but a number of the surrounding ECMWF grid points have surface type “sea” (or vice versa), these grid points shall be disregarded in the spatial interpolation. Otherwise, coastal features will be apparent in the final product. Figure 2 shows a schematic of this process.

In case, however, that all surrounding ECMWF grid points differ in their surface type from the pixel's surface type (e.g. small islands or small lakes or rivers), all four surrounding grid points have to be used.

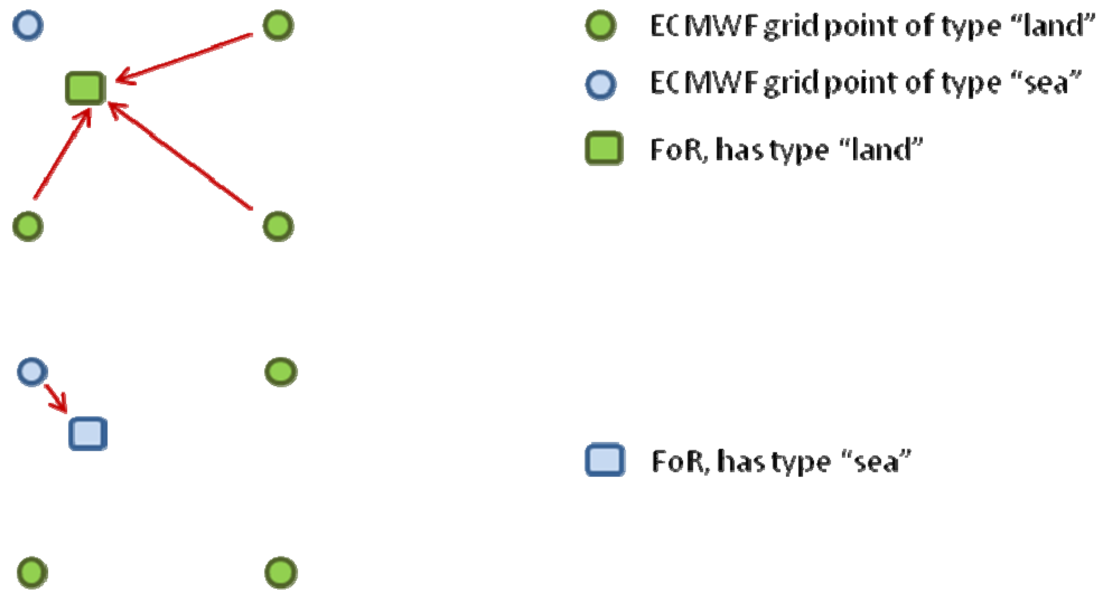

Figure 2: Schematic illustration of the use of forecast data depending on the FoR and the forecast grid surface type. Only the forecast data of the same surface type shall be used, as illustrated for the "land" case (top) and the "sea" case (bottom). The arrows denote which ECMWF grid points shall be used in these cases.

3.4.3 Ancillary Static Data

3.4.3.1 Information on Surface Emissivity

The RTM calculations need information on the surface emissivity for all L channels. The following cases are discriminated:

Processing Version I – full GII and TOZ retrieval over cloud free surface:

A-1: The FoR's predominant surface type is sea: RTTOV offers an internal calculation of the sea surface emissivity, depending on the satellite view angle. The results of these calculations shall be used (e.g. in RTTOV-9.1 this is the parameter CALCEMIS which has to be set to .TRUE.)

A-2: The FoR's predominant surface type is land. In this case, the available pixel-based emissivity data for all L channels shall be used. These data are constant over a certain period (typically a month), so the processing has to allow for a possible time dependence in this input dataset. Also, the pixel based emissivity shall be averaged over the cloud free pixels in the respective FoR.

Processing Version II – TOZ retrieval over clouds:

The cloud emissivity is parameterised as follows:

$$\varepsilon(\mathrm{ch}) = a_0(\mathrm{ch}) + \frac{a_1(\mathrm{ch})}{\cos\zeta_{sat}} + \frac{a_2(\mathrm{ch})}{\cos^2\zeta_{sat}} \qquad \mathbf{(3)}$$

where
ε: emissivity
ch: index for channel (1 to L)
ζ_{sat}: satellite viewing angle
a_0, a_1, a_2: channel dependent, pre-calculated regression coefficients

Section 3.5.1 describes how this cloud emissivity information shall be used within the processing.

3.4.3.2 Covariance Matrix of First Guess Errors (S_x)

The statistical error of the background is represented by the matrix $\mathbf{S}_x$. This (3M+1) by (3M+1) element matrix describes the covariance of the background errors between parameters at different levels. The pairs of errors for temperature, humidity, ozone and skin temperature are assumed to be uncorrelated und thus set to 0. The levels M correspond to the RTTOV pressure levels. The matrix for Version I is schematically shown in Figure 2. Version II would have the identical matrix, with only the exception that the last (bottom right) matrix element is no longer the skin temperature covariance (which is typically 15K·15K), but is now the covariance of the cloud top pressure. A value of 200 hPa * 200 hPa is used in this case.

Units in the covariance matrix of first guess errors have to correspond to the units of the observation vector (K^2 for temperatures, $ppmv^2$ for gases, hPa^2 for cloud height).

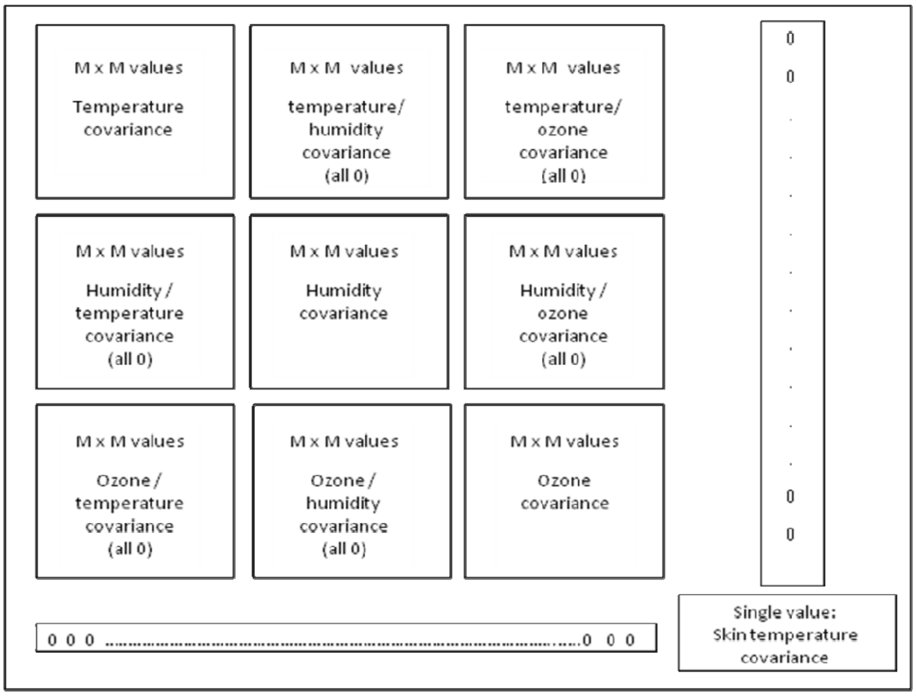

Figure 2: Schematic of the error covariance matrix $\mathbf{S}_x$ for Version I processing.

3.4.3.3 Observation and Radiation Model Errors (S_ε)

The statistical errors of the observed brightness temperatures and the errors of the radiation model are represented by the matrix $\mathbf{S}_\varepsilon$. The elements describe the covariance of the brightness temperature error of the instrument, and an assumed uncertainty of the radiation model is added to that value. As the covariance of any two channels is not known, but probably uncorrelated, they are set to 0, so the matrix has only diagonal non-zero elements, representing single channel errors. These errors are simply assumed to be the instrument noise figures for the respective channel. The (assumed) error of the radiation model (e.g. a value of typically 0.2 K) is added (in a squared sense) to these diagonal elements with the implicit assumption that instrument and model noise are uncorrelated. The matrix is of size L by L, where L is the number of channels used in the processing. The matrix remains unchanged between the processing versions I and II.

3.5 Detailed Description

Once all input data is available and properly averaged and interpolated for a single FoR, the physical retrieval process can start, which consists of five main tasks

(a) Run the radiative transfer forward model to compute the simulated brightness temperatures for a given observation vector x_n
(b) Compare RTM temperatures to measurements to assess quality of retrieval iteration
(c) Run the radiative transfer K-model (Jacobians) to compute the matrix $\mathbf{K}_n$
(d) Solve equation (1)
(e) Update the observation vector x_n

3.5.1 RTM Forward Model

Version I processing – cloud free case:

The RTM forward model of RTTOV (in RTTOV-9.1 this is the module rttov_direct) provides the clear sky brightness temperatures for the provided temperature profile (observation vector x_0). The processing has to make sure that the corresponding variable structure in RTTOV, describing the profile, is properly populated, and has the correct units.

Note: In RTTOV-9.1, the structure variable is *profiles*, where

profiles % t(1:M)	are the air temperatures in K
profiles % q(1:M)	are the humidities in ppmv
profiles % o3(1:M)	are the ozone values in ppmv
profiles % skin % t	is the surface skin temperature in K
profiles % skin % p	is the surface pressure in hPa
profiles % skin % surftype =	0 (for land), = 1 (for sea)
profiles % s2m % t	is the 2m temperature (can be proxied by lowest level air temperature), in K
profiles % s2m % q	is the 2m humidity (can be proxied by the lowest level humidity), in ppmv
profiles % s2m % o	is the 2m ozone (can be proxied by the lowest level ozone), in ppmv

profiles % zenangle satellite viewing angle in degrees
profiles % cfraction = 0.0, cloud fraction

The results of the forward model are the brightness temperatures for the cloud free case, in RTTOV-9.1 these are stored in *radiance % bt_clear(1:L)* for all channels L, and they constitute the data for $T_{B,n}$ in equation (1).

Version II processing – cloudy case:

The same forward model as for the Version I processing is called, and only two parameters are changed in the input structure *profiles*:

profiles % cfraction = 1.0 – cloud fraction is set to 1 to get the cloudy case
profiles % ctp = first guess cloud pressure, in hPa

Section 3.4.2.2 describes how to obtain a first guess cloud pressure value.

The RTM output for the cloudy case has to be corrected for the actual cloud emissivity (as parameterised in section 3.4.3.1):

The radiance r(ch,m) at the top of the atmosphere, for channel ch, and with a cloud of emissivity ε at layer m is composed of:

(a) The emission from the cloud, multiplied by the atmospheric transmission above layer m:

$$\varepsilon(\mathrm{ch})\ B_{\mathrm{ch}}\left[T(m)\right]\ \tau_a(\mathrm{ch}, m)$$

$\varepsilon(ch)$: channel specific cloud emissivity for channel ch
$B_{ch}[T(m)]$: spectral blackbody radiance for channel ch at level m, which has air temperature T(m)
$\tau_a(ch,m)$: atmospheric transmission in channel ch above level m

(b) Downwelling radiation reflected by the cloud

$$(1-\varepsilon(\mathrm{ch}))\ r_{\mathrm{down}}(\mathrm{ch}, m)\ \tau_a(\mathrm{ch}, m)$$

$1-\varepsilon(ch)$: reflectivity in channel ch
$r_{down}(ch,m)$: downwelling radiation for channel ch at level m
$\tau_a(ch,m)$: atmospheric transmission in channel ch above level m (as above)

(c) Contribution from the layers above the cloud, which can be inferred from

$$r_{\mathrm{top,overcast}}(\mathrm{ch}, m) - B_{\mathrm{ch}}\left[T(m)\right]\ \tau_a(\mathrm{ch}, m)$$

$r_{top,overcast}(ch,m)$: outgoing radiance at the top of the atmosphere, for channel ch, for a cloud of ε=1 at level m,

$B_{ch}[T(m)]$ and $\tau_a(ch,m)$ are defined as above.

The standard RTTOV output of the forward calculations provide all the necessary terms $\tau_a(ch,m)$, $r_{top,overcast}(ch,m)$, $r_{down}(ch,m)$, and B_{ch} $[T(m)]$ can be calculated from Planck's formula, summing up terms (a), (b) and (c) provides the radiance at the top of the atmosphere, if a cloud of the given emissivity is at level m.

This implies, that after the call to the RTM forward model, the resulting cloudy radiances have to be corrected according to:

$$r_{final}(ch) = \varepsilon(c)\, B_{ch}[T(m)]\, \tau_a(ch,m) + (1-\varepsilon(ch))\, r_{down}(ch,m)\, \tau_a(ch,m) + r_{top.overcast}(ch,m) - b_{ch}[T(m)]\, \tau_a(ch,m) \tag{4}$$

RTTOV provides as output (in version 9.1):

transmission % tau(c,m)	representing $\tau_a(ch,m)$
radiance % down(c,m)	representing $r_{down}(ch,m)$
radiance % overcast(c,m)	representing $r_{top,overcast}(ch,m)$

The such corrected radiances $r_{final}(c)$ need to be converted to brightness temperatures T_{Bn} in equation (1) (for details on the radiance to brightness temperature conversion, see e.g. the realisation within the RTTOV software).

3.5.2 Condition to Terminate Iterative Process

The iterative process is terminated if the simulated brightness temperatures $T_{B,n}$ are close to the observed and bias corrected temperatures T_B. The actual termination criterion is the root mean square difference between the two sets of temperatures

$$RMS = \frac{\Sigma\left(T_B - T_{B,m}\right)^2}{\text{number of channels}} \tag{5}$$

The summation is here done over the channels m, where for the Version I processing all L channels are used, and for the Version II processing only a selected subset of channels, typically IR9.7, IR10.8 and WV6.2 (i.e. in this case the "number of channels in the denominator of equ. (5) is 3)

If RMS is lower than a certain threshold (which may be different for the version I and II processing), the atmospheric profile of the iteration step n is taken as the retrieved profile (obviously, this can also happen in step n=0, i.e. the first guess profile already well fits the satellite measurements, which is the easiest case, where the processing does not even have to solve equation (1)).

In the (rare) case that the RMS never meets the threshold, the iteration process has to be terminated as a retrieval failure case after a maximum number of iterations (typically 5).

Also, if the RMS in iteration step (n+1) is larger than the RMS of iteration step n, this can be regarded as a failure and the retrieval can be stopped.

In summary, the iterative process is terminated if

(a) RMS meets the threshold criterion → profile of the current iteration step is the retrieval result
(b) Maximum number of allowed iteration steps is reached → failed retrieval
(c) RMS(n+1) > RMS(n) → failed retrieval

3.5.3 RTM K-Model

The K-model of RTTOV provides the Jacobian matrix $\mathbf{K}_n$ for the iteration step n (in RTTOV-9.1 this is the module rttov_k). This matrix describes the change of the radiation field at the top of the atmosphere with a changed atmospheric profile:

$$\mathbf{K}_n(c,m) = \frac{\partial T_{B,n}(c)}{\partial x_n(m)} \qquad \textbf{(6)}$$

where c denotes a channel number and m denotes an element of the profile vector x_n. The matrix has thus L columns and (3M+1) rows – M for temperature, M for humidity, M for ozone, and 1 for the skin temperature resp. cloud top pressure, and L is the number of channels.

In RTTOV-9.1, $\mathbf{K}_n$ is provided by module rttov_k, which is called with the same input as the RTM forward model rttov_direct (see section 3.5.1).

Version I processing – cloud free case:

The K-Model provides the Jacobians for air temperature (units K/K), for humidity (units K/ppmv), for ozone (units K/ppmv), for surface skin temperature (units K/K) and the structure of final $\mathbf{K}_n$ matrix is shown in Figure 3:

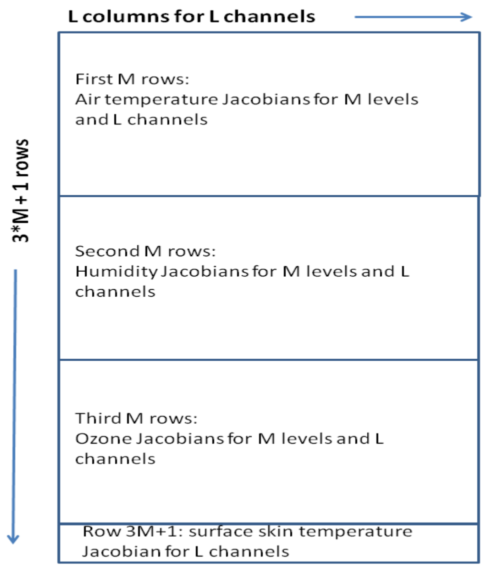

Figure 3: Structure of the final Jacobian matrix $\mathbf{K}_n$ for the Version I processing

Version II processing – cloudy case:

In this case, the structure of the final $\mathbf{K}_n$ matrix is (Figure 4):

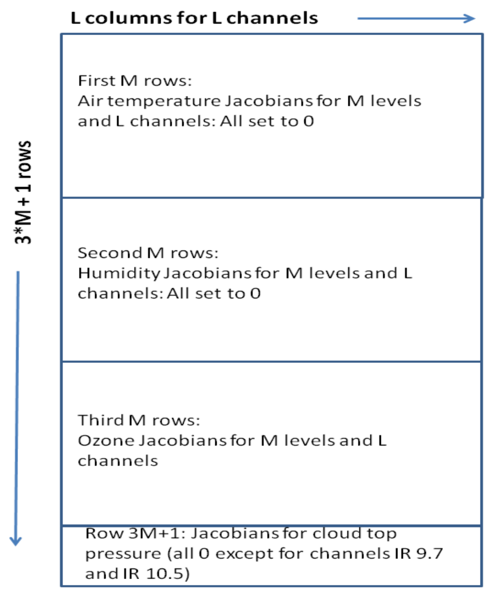

Figure 4: Structure of the final Jacobian matrix $\mathbf{K}_n$ for the Version II processing

The largest differences to the Version I matrix $\mathbf{K}_n$ are
(a) The Jacobians for temperature are all set to 0
(b) The Jacobians for humidity are all set to 0
(c) The last row is changed from the surface skin temperature Jacobians to cloud top pressure Jacobians (details see below), but only for channels IR 9.7 and IR 10.8, for all other channels these are set to 0

These settings imply that only the IR 9.7 and the IR 10.8 channels will be of relevance within the retrieval, i.e. only these two channels may actually contribute to a changed ozone profile together with a changed cloud top pressure (the latter only being important as a lower boundary condition, not as a product in itself). The other channels, however, are still used in the monitoring of the minimisation success, i.e. in the computation of the RMS brightness temperature difference (section 3.5.2).

The Jacobians for the cloud top pressure (units K/hPa) are not a direct output of the RTTOV K-model, and they are calculated as follows:

(a) Get the first guess cloud level *icloud* (as described in section 3.4.2.2). *icloud* refers to a standard level as defined within RTTOV
(b) From the RTM forward model output, get the top of atmosphere radiances for clouds in level *icloud* ± a certain (small) number (e.g. 3) = *icloud1* and *icloud2*, but not lower than the surface
(c) The cloudy radiances in levels *icloud1* and *icloud2* have to be converted to brightness temperatures, for channels IR 9.7 and IR 10.8, yielding $T_{B,cloud}(9.7)$ and $T_{B,cloud}(10.8)$ for both levels
(d) The levels *icloud1* and *icloud2* are associated with pressures *p(icloud1)* and *p(icloud2)*
(e) The cloud top pressure Jacobian can then be approximated by

$$\frac{T_{B,cloud}(\text{cloud at level icloud1}) - T_{B,cloud}(\text{cloud at level icloud2})}{p(\text{level icloud1}) - p(\text{level icloud2})}$$

separately for channels IR 9.7 and IR 10.8. *icloud1* and *icloud2* are defined such that p(icloud1) > p(icloud2)

3.5.4 Solution of Equation (1)

Once all the satellite observations, atmospheric profile, error and Jacobian matrices are available, equation (1) can be solved for the next iteration step n+1:

$$x_{n+1} = x_0 + (\mathbf{S}_x^{-1} + \mathbf{K}_n^T \cdot \mathbf{S}_\varepsilon^{-1} \cdot \mathbf{K}_n)^{-1} \times \mathbf{K}_n^T \cdot \mathbf{S}_\varepsilon^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0) \right] \qquad \textbf{(7)}$$

Inspection of equation (1) shows that it involves the inversion of a large matrix, namely

$$\mathbf{S}_x^{-1} + \mathbf{K}_n^T \cdot \mathbf{S}_\varepsilon^{-1} \cdot \mathbf{K}_n \qquad \textbf{(8)}$$

which is of size (3M+1) by (3M+1). Equation (1), however, can be rearranged to

$$x_{n+1} = x_0 + \mathbf{S}_x \cdot \mathbf{K}_n^T \cdot \left(\mathbf{K}_n \cdot \mathbf{S}_x \cdot \mathbf{K}_n^T + \mathbf{S}_\varepsilon \right)^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0) \right] \qquad \textbf{(9)}$$

which only involves the inversion of a much smaller matrix

$$\mathbf{K}_n \cdot \mathbf{S}_x \cdot \mathbf{K}_n^T + \mathbf{S}_\varepsilon \qquad \textbf{(10)}$$

which is of size L by L, L being the number of channels..

The aim of solving equation (7) is to find an expression of $x_{n+1} - x_0$, i.e. rewrite equation (7) to

$$x_{n+1} - x_0 = \mathbf{S}_x \cdot \mathbf{K}_n^T \cdot \left(\mathbf{K}_n \cdot \mathbf{S}_x \cdot \mathbf{K}_n^T + \mathbf{S}_\varepsilon\right)^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0) \right] \qquad \textbf{(11)}$$

This involves the following computational steps:

(a) Transpose matrix $\mathbf{K}_n$, yielding	$\mathbf{K}_n^T$	[size (3M+1) by (L)]
(b) Perform matrix multiplication	$\mathbf{S}_x \cdot \mathbf{K}_n^T = \mathbf{W}_1$	[size (3M+1) by (L)]
(c) Perform matrix multiplication	$\mathbf{K}_n \cdot \mathbf{W}1$	[size (L) by (L)]
(d) Add matrix $\mathbf{S}_\varepsilon$	$\mathbf{K}_n \cdot \mathbf{W}_1 + \mathbf{S}_\varepsilon = \mathbf{W}_2$	[size (L) by (L)]
(e) Invert $\mathbf{W}_2$ yielding	$\mathbf{W}_2^{-1}$	[size (L) by (L)]
(f) Perform matrix multiplication	$\mathbf{K}_n^T \cdot \mathbf{W}_2^{-1} = \mathbf{W}_3$	[size (3M+1) by (L)]
(g) Perform matrix multiplication	$\mathbf{S}_x \cdot \mathbf{W}_3 = \mathbf{W}_4$	[size (3M+1) by (L)]
(h) Compute	$\mathbf{K}_n \cdot (x_n - x_0) + T_B - T_{B,n} = v$	[size (L)]
(i) Get final result	$\Delta x_{n+1} = x_{n+1} - x_0 = \mathbf{W}_4 \cdot v$	[size (3M+1)]

3.5.5 Update Observation Vector x

Once the new vector Δx_{n+1} is obtained, the observations of temperature, humidity, ozone, surface skin temperature (resp. cloud top height) can be updated according to

$$x_{n+1} = x_0 + \Delta x_{n+1} \qquad \textbf{(12)}$$

i.e. the new iteration x_{n+1} is obtained by simply adding the $(x_{n+1}-x_0) = \Delta x_{n+1}$ value to the background x_0.

Version I processing – cloud free case:

Equation (9) provides the air temperatures $x_n(1{:}M)$ in units K, the humidities $x_n(M+1{:}2M)$ in ppmv, the ozone values $x_n(2M+1{:}3M)$ in ppmv, and the surface skin temperature $x_n(3M+1)$ in K.

Before this updated profile is used in the next iteration (starting with the RTM forward calculations), some physical constraints are applied:

(a) Relative humidity shall not exceed 100%: From the temperature and humidity, the relative humidity can be derived (for details, see section 3.5.7). For levels where this exceeds 95%, the relative humidity is set to the fixed value 95%, from which the specific humidity in ppmv is inferred. In order to have a correct value for Δx_{n+1} for the next iteration step, this is set to

$$\Delta x_{n+1} = x_{n+1}(\text{corrected for high humidity}) - x_0 \qquad \textbf{(13)}$$

for the relevant levels between M+1 and 2M, x_0 being the background value, which for Version I is the first guess atmospheric profile/surface skin temperature.

(b) Humidity values should not be less than 0 ppmv: In this case the humidity values are simply set back to the first guess, and the respective Δx_{n+1} for the affected levels is set to 0.
(c) The updated ozone profile has to be within some maximum and minimum constraints (from within RTTOV, which defines $ozone_{min}$ and $ozone_{max}$ values for each RTTOV level). Ozone values below the minimum or above the maximum for the respective level are set to the minimum or maximum value, and Δx_{n+1} is changed to

$$\Delta x_{n+1} = x_{n+1}(\text{set to min/max ozone}) - x_0 \qquad \textbf{(14)}$$

Note: In case the profile x_{n+1} is changed because of these physical constraints, it is important to update Δx_{n+1} as this is needed in the next iteration step!

Version II processing – cloudy case:

In this case, equation (9) only provides updates for the ozone values $x_{n+1}(2M+1:3M)$, as the respective Δx_{n+1} values for indices (1:2M) are all 0, because the relevant Jacobians are 0. Ozone values are updated according to the method outlined above (Version I processing), also including the same constraints as outlined in (c) above.

The updated cloud top height is also derived according to equation (9) (for index (3M+1), where care has to be given to the meaning of x_0 in this casespecial case – x_0 is the cloud background pressure, not the first guess.

3.5.6 Definition of GII Indices, Precipitable Water and Total Column Ozone

3.5.6.1 Lifted Index

$$LI = T - T^{\text{lifted from surface}} \text{ at 500 hPa} \qquad \textbf{(15)}$$

From the derived temperature profile, the air temperature at 500 hPa needs to be interpolated between the adjacent pressure levels (interpolation needs to be done logarithmically with pressure). This comprises the first T^{air} term in equation (12).

Concerning the second term, the characteristics of the air parcel which is to be theoretically lifted to 500 hPa, is defined as the average temperature and humidity content of the lowest 100 hPa in the atmosphere. The averaging in temperature and humidity shall be done linearly with pressure. The air parcel with such defined temperature and humidity is then lifted adiabatically from the surface to the lifting condensation level, and lifted moist adiabatically from the lifting condensation level to 500 hPa (see 3.5.7.7). The parcel temperature at 500 hPa is the second term in equation (12), $T^{\text{air, lifted from surface}}$, and the Lifted Index is simply the difference of these two terms.

In case the surface pressure is below 500 hPa, the K-Index is not defined.

3.5.6.2 K-Index

$$KI = (T^{(850)} - T^{(500)}) + TD^{(850)} - (T^{(700)} - TD^{(700)}) \qquad \textbf{(16)}$$

From the derived temperature profile, the air temperatures at 850, 700 and 500 hPa need to be interpolated from the adjacent respective pressure levels (interpolation needs to be done logarithmically with pressure). This defines the terms $T^{(850)}$, $T^{(700)}$ and $T^{(500)}$ in equation (13). The dew point temperatures at 850 and 700 hPa need to be interpolated from the adjacent respective pressure levels (interpolation needs to be done logarithmically with pressure for the temperatures, linear with pressure for the humidities). This defines the terms $TD^{(850)}$ and $TD^{(700)}$ in equation (13). The K-Index is then computed according to equation (13). All temperature values in equation (13) are expressed in Kelvin, the K-Index, however, is commonly expressed in deg Celsius, so 273.15 needs to be subtracted from the final value of equation (13).

In case the surface pressure is below 850 hPa, the K-Index is not defined.

Section 3.5.7 will describe in more detail the necessary thermodynamic functions that shall be used within these calculations.

3.5.6.3 KO-Index

$$KO = 0.5\,(\Theta_e^{(500)} + \Theta_e^{(700)} - \Theta_e^{(850)} - \Theta_e^{(1000)}) \qquad \textbf{(17)}$$

From the derived profile data, the equivalent potential temperatures at 500, 700, 850 and 1000 hPa need to be derived from the respective temperatures T, humidities q and pressure values p. T and q need to be interpolated from the adjacent respective pressure levels (interpolation needs to be done logarithmically with pressure for T, linear with pressure for q). The definition of Θ_e is given in section 3.5.7.6. This defines the terms $\Theta_e^{(500)}$, $\Theta_e^{(700)}$, $\Theta_e^{(850)}$ and $\Theta_e^{(1000)}$ in equation (17).

3.5.6.4 Maximum Buoyancy

$$MB = \Theta_e^{max} - \Theta_e^{min} \qquad \textbf{(18)}$$

Θ_e^{max} is the maximum equivalent potential temperature between the surface and 850 hPa height, Θ_e^{min} is the minimum equivalent potential temperature between 300 and 700 hPa height. The Θ_e values of the surface level and of the 850, 700 and 300 hPa height need to be derived from the respective temperatures T, humidities q and pressure values p. T and q need to be interpolated from the adjacent respective pressure levels (interpolation needs to be done logarithmically with pressure for T, linear with pressure for q). The definition of Θ_e is given in section 3.5.7.6. The Θ_e values for the levels between surface and 850 hPa, and between 700 and 300 hPa can be directly derived from the profile data. The maximum value between the surface and 850 hPa defines Θ_e^{max}, the minimum value between 700 and 300 hPa defines Θ_e^{min}, and MB is simply computed as the difference between these two terms.

3.5.6.5 Layer Precipitable Water (LPW)

LPW shall contain the vertically integrated humidity in three layers. Layer boundaries are

(a) Surface to 850 hPa

(b) 850 to 500 hPa
(c) 500 hPa to top of atmosphere

Humidity values (mixing ratio, expressed in kg/kg) shall first be interpolated to the layer boundaries, 850 and 500 hPa, where the interpolation is linear with pressure between the respective pressure levels.

The vertical integration shall then be done according to

$$LPW_i = \frac{1}{g} \int_{p1}^{p2} q(p)\, dp \tag{19}$$

where:

LPW_i: LPW of a specific layer i
g: earth gravitational acceleration
q(p): value of water vapour mixing ratio (in kg/kg) at pressure level p
p1, p2: pressure boundaries of the layer i

LPW is expressed in kg/m^2.

In practice, the integration is done as a summation of the available pressure levels:

$$LPW_i = \frac{1}{g} \sum \overline{q}(p)\, \Delta p \tag{20}$$

$\overline{q}(p)$ is the average humidity in the layer defined by the pressure difference Δp; the summation is done over the respective pressure levels for each LPW layer.

3.5.6.6 Total Precipitable Water (TPW)

TPW is simply the sum of the three layer precipitable water values:

$$TPW = LPW_1 + LPW_2 + LPW_3 \tag{21}$$

3.5.6.7 Total Column Ozone (TOZ)

TOZ is the vertically integrated ozone, where the vertical integration is done between the surface and the top of the atmosphere.

$$TOZ = \frac{1}{g} \int_{p(surface)}^{p(top\,level)} o_3(p)\, dp \tag{22}$$

where:

g: earth acceleration of gravity
$o_3(p)$: value of ozone mixing ratio (in kg/kg) at pressure level p

In practice, the integration is done as a summation of the available pressure levels:

$$\mathrm{TOZ} = \frac{1}{g} \sum \bar{o}_3(p)\,\Delta p \qquad \mathbf{(23)}$$

$\bar{o}_3(p)$ is here the average ozone in the layer defined by the pressure difference Δp; the summation is done over all pressure levels of the vertical profile

TOZ according to equations (17) and (18) is of unit kg/m^2 (provided that pressure p is expressed in Pa).

As TOZ is commonly expressed in Dobson Units, the integral has to be divided by 21.4E-06:

$$\mathrm{TOZ(Dobson\ Units)} = \mathrm{TOZ(kg/m^2)} / 21.4\mathrm{E}\text{-}06 \qquad \mathbf{(24)}$$

3.5.7 Thermodynamic Formulae

A number of thermodynamic formulae are used in the GII/TOZ processing, which are described in this section.

3.5.7.1 Conversion between Units ppmv and Mixing Ratio (kg/kg)

For humidity, the conversion factors between units ppmv and mixing ratio expressed in (kg/kg) are:

Mixing ratio to ppmv: 1.60771704E+06
ppmv to mixing ratio: 1./1.60771704E+06

For ozone, the respective values are

mixing ratio to ppmv: 6.03504E+05
ppmv to mixing ratio: 1./6.03504E+05

e.g. a 0.01 kg/kg humidity mixing ratio corresponds to 0.01 * 1.60771704E+06 = 1.60771704E+05 ppmv.

3.5.7.2 Saturation Vapour Pressure for a Given Temperature T

The saturation water vapour pressure E(T) depends on air temperature only and can be expressed as

$$E(T) = 6.11 \cdot 10^{7.5\cdot(T-273.15)/(T-273.15\ +237.3)} \qquad \mathbf{(25)}$$

Temperature T is expressed in units K, and the resulting vapour pressure is in units hPa.

3.5.7.3 Relative Humidity for a Given Pressure, Temperature and Mixing Ratio

For a given pressure p, a humidity mixing ratio q and a temperature T, the relative humidity RH is defined according to

$$RH = \frac{e \cdot 100}{E(T)} \tag{26}$$

RH is in %, v is the local vapour pressure in hPa and E(T) the saturation vapour pressure as defined in section 3.5.7.2. can be obtained via

$$e = \frac{q \cdot p}{(0.622 + 0.378\ q)} \tag{27}$$

The humidity mixing ratio q is expressed in kg/kg, pressure p and saturation vapour pressure in hPa, temperature in K. The resulting vapour pressure e is then also of unit hPa.

3.5.7.4 Mixing Ratio for a Given Pressure, Temperature and Relative Humidity

For a given pressure p, relative humidity RH and temperature T, the mixing ratio q is defined according to

$$q = \frac{0.622\ e}{p - 0.378\ e} \tag{28}$$

e is the local vapour pressure and is obtained via

$$e = \frac{E(T) \cdot RH}{100} \tag{29}$$

from the saturation vapour pressure E(T) and temperature T (see section 3.5.7.2). Temperature is expressed in K, pressure p in hPa, relative humidity RH in %. The resulting mixing ratio is of unit kg/kg.

3.5.7.5 Calculation of Dew Point Temperature

An empirical formula is used for the dew point calculations. For a given level with temperature T, saturation vapour pressure E(T) and relative humidity RH, the dew point TD is defined according to

$$TD = \frac{243.5 \cdot A - 440.8}{19.48 - a} + 273.15 \tag{30}$$

with

$$a = \ln\left(\frac{E(T) \cdot RH}{100}\right) \tag{31}$$

E(T) is given by equation (20).

3.5.7.6 Calculation of the Equivalent Potential Temperature

The **equivalent potential temperature** Θ_e is the temperature a parcel of air would reach if all the water vapour in the parcel were to condense, releasing its latent heat, and the parcel was brought adiabatically to the standard reference pressure of 1000 hPa.

For an air parcel, characterised by p, T and q, the equivalent potential temperature is computed from:

$$\theta_e = \theta\, e^{b1 \cdot b2} \tag{32}$$

θ is the potential temperature of T, defined by

$$\theta = T \left(\frac{1000}{p_{sfc}} \right)^{R/c_p} \tag{33}$$

b1 and b2 are empirical coefficients and are derived according to

$$\begin{aligned} b1 &= \frac{3.376}{T_{lift}} - 0.00254 \\ b2 &= 1000 \cdot q \cdot (1 + 0.81 \cdot q) \end{aligned} \tag{34}$$

T_{lift} is the lifting condensation level temperature as defined in section 3.5.7.7.

3.5.7.7 Specific Functions Needed for the Lifted Index Calculations

For the Lifted Index, the vertical lapse rate for the (theoretically) lifted near-surface air particle is the dry adiabatic lapse rate until the lifting condensation level is reached, and the moist adiabatic lapse rate beyond this level up to 500 hPa. The near-surface air parcel is defined as the average temperature and humidity over the lowest 100hPa above the surface together with the surface pressure – these variables are in the following denoted as T_{sfc}, q_{sfc}, p_{sfc}.

The **lifting condensation level temperature** T_{lift} is obtained through the empirical formula

$$T_{lift} = \frac{1}{\dfrac{1}{T_{sfc} - 55} - \dfrac{\ln(RH_{sfc}/100)}{2840}} \tag{35}$$

RH_{sfc} is the relative humidity of this air parcel, expressed in %, derived from T_{sfc} and p_{sfc} according to equations (21) and (22).

The **pressure of the lifting condensation level** p_{lift} is defined as the pressure, where the near-surface air parcel, having temperature T_{sfc}, reaches the lifting condensation temperature T_{lift}

during a dry adiabatic process. The lifting condensation pressure can thus be obtained from the dry adiabatic formula (Poisson's equation):

$$p_{lift} = \frac{p_{sfc}}{\left(\frac{T_{sfc}}{T_{lift}}\right)^{R/c_p}} \quad \textbf{(36)}$$

p_{lift} is given in units hPa. R is the gas constant for moist air, c_p is the specific heat for moist air. R and c_p depend on the near-surface humidity q_{sfc} and are computed according to

$$\begin{aligned} R &= (1 + 0.608\,q_{sfc}) \cdot 287.04 \\ c_p &= (1 + 0.887\,q_{sfc}) \cdot 1005.7 \end{aligned} \quad \textbf{(37)}$$

For the computation of the Lifted Index, two different cases now need to be distinguished:

(a) $p_{lift} \leq 500$ hPa (which in reality almost never happens)
(b) $p_{lift} > 500$ hPa

In the rare event of case (a), this implies that the temperature of the near-surface air parcel, displaced to 500 hPa, simply follows the dry adiabat, so can be easily inferred from

$$T^{\text{air, lifted from surface}} = T_{sfc} \left(\frac{500}{p_{sfc}}\right)^{R/c_p} \quad \textbf{(38)}$$

$T^{\text{air, lifted from surface}}$ here refers to the respective term in equation (12).

Usually, the lifting condensation level is well below the 500 hPa height (i.e. $p_{lift} > 500$ hPa). In this case (b), the air parcel has to follow the moist adiabat between p_{lift} and 500 hPa.

As a first step, the **equivalent potential temperature** of the near-surface air parcel, characterised by p_{sfc}, T_{sfc} and q_{sfc}, is computed according to equation (27).

In the next step, the **final air temperature, lifted to 500 hPa from the surface** is computed as a difference between two temperatures:

$$T^{\text{air, lifted from surface}} = T1 - T2 \quad \textbf{(39)}$$

T1 is the temperature of θ_e (equation (31)), if dry adiabatically displaced to 500 hPa:

$$T1 = \frac{\theta_e}{\left(\frac{1000}{500}\right)^{R_{dry}/c_{p,dry}}} \quad \textbf{(40)}$$

(obviously, 1000/500 = 2, numbers were put in for reference to Poisson's equation). R_{dry} and $c_{p,dry}$ are the gas constant and specific humidity for dry air (q = 0 in equation (29))

T2 is computed using an empirical regression scheme. The following steps are involved:

(a) compute $t = T1 - 293.16$
(b) In case $t < 0$:

$$T2 = \frac{15.13}{P^4} \qquad \textbf{(41)}$$

(c) In case $t \geq 0$:

$$T2 = \frac{29.93}{P^4} + 0.96 \cdot t - 14.8 \qquad \textbf{(42)}$$

In both equations (41) and (42) the term P is a third order polynomial of t:

$$P = 1 + c_1 t + c_2 t^2 + c_3 t^3 \qquad \textbf{(42)}$$

Values of c_1, c_2, c_3 depend on the value of t:

	$t \leq 0$	$t > 0$
c_1	-8.8416605 E-03	+3.6182989 E-03
c_2	+1.4714143 E-04	-1.3603273 E-05
c_3	-9.6719890 E-07	+4.9618922 E-07

This final $T^{\text{air, lifted from surface}}$ of equation (39), is used in equation (12) for the Lifted Index.

3.6 Output Description

The output of the GII processing are:

- The Lifted Index, unit K, according to equation(12)
- The K-Index, unit °C, according to equation (13)
- Layer Precipitable Water, lower troposphere, unit kg/m^2, according to equation (14)
- Layer Precipitable Water, middle troposphere, unit kg/m^2, according to equation (14)
- Layer Precipitable Water, upper troposphere, unit kg/m^2, according to equation (14)
- Total Precipitable Water, unit kg/m2, according to equation (16)
- Total Ozone, in Dobson Units, according to equations (17) and (19)

The output is generated for each FoR. In case a FoR is more than just a single pixel, the fraction of cloud free pixels used within the FoR can be added as a quality information. This will automatically also flag the special case of Version II processing where TOZ is derived over cloudy areas (cloud free fraction = 0.0).

As the K-Index (and theoretically also the Lifted Index) can be undefined (in case of surface pressure below 850hPa or 500hPa, the final product has to allow "undefined" as output for each of the two parameters.

For the final disseminated product it must be kept in mind that the TOZ values will cover many more FoRs than the full GII output, because of the special Version II cloudy processing. TOZ might thus have to go into a different dissemination data stream.

Meaningful limits for the product entries (e.g. for BUFR compression) are:

K-Index between -30 and +70 °C
Lifted Index between -20 and +40 K
TPW, LPW between 0 and 100 kg/m^2
TOZ between 0 and 700 DU

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